

Dual Fermion Method for Disordered Electronic Systems

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While the coherent potential approximation (CPA) is the prevalent method for the study of disordered electronic systems, it fails to capture non-local correlations and Anderson localization. To incorporate such effects, we extend the dual fermion approach to disordered non-interacting systems using the replica method. Results for single- and two- particle quantities show good agreement with cluster extensions of the CPA; moreover, weak localization is captured. As a natural extension of the CPA, our method presents an alternative to the existing cluster theories. It can be used in various applications, including the study of disordered interacting systems, or for the description of non-local effects in electronic structure calculations.

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Introduction.- Disorder, due to doping, impurities or structural defects, is a common feature of many materials, and may play a crucial role in determining transport properties. The coherent potential approximation (CPA) is the most common theoretical method used to study disordered systems [1]. While the CPA is a successful single-site theory of disorder it misses, by construction, non-local effects including Anderson localization [2]. Cluster extensions of the CPA, such as the Molecular CPA [3] and the Dynamical Cluster Approximation (DCA) [4], capture non-local correlations within the cluster [5]; however, Anderson localization is still missing.

The Dual Fermion (DF) formalism [6], originally developed for clean interacting systems, is complementary to these cluster approaches. It treats local correlations explicitly in the “impurity” solver, and non-local correlations perturbatively. So, if a geometric series of relevant diagrams are included, it has the potential to capture localization. Here we present such a DF method for disordered systems.

The DF formalism is based on a set of auxiliary variables (dual fermions) which are introduced into the path integral representation of the lattice partition function via a canonical transformation [7, 8]. It maps the lattice onto an impurity embedded in a self-consistently determined dual fermion lattice. The DF lattice problem is treated via a perturbation theory involving the DF bare Green function, which is the difference of the lattice and impurity Green functions, and the impurity full vertex as the effective bare DF interaction [9]. These features are elegantly incorporated in Rubtsov’s DF formalism [6].

For systems with disorder, the DF mapping has to be done differently. In particular, as observable quantities are calculated by derivatives of the free energy, the DF formalism for the disorder case then needs to be constructed from the disorder averaged $\langle \ln Z \rangle_{av}$ instead of from the partition function Z as in [6].

In this Letter we employ the replica method [10] to deal with such averaging. We extend the DF method to systems with disorder, and construct the DF mapping directly on the Green function. We demonstrate that our method shows remarkable agreement for the single-particle Green function with the results obtained from large cluster DCA calculations. Moreover, our disorder DF can account for weak localization in the conductivity. This scheme presents a powerful alternative to the existing cluster extensions of CPA, with a broad venue of applications, including the possibility of treating both electron-electron interactions and disorder on equal footing, or replacing the CPA in electronic structure calculations.

Method.- The simplest model of disordered electrons is the Anderson model. Its Hamiltonian is

$$H = - \sum_{\langle ij \rangle} t_{ij} (c_i^\dagger c_j + h.c.) + \sum_i V_i n_i, \quad (1)$$

where $4t = 1$ sets the energy unit, and the local potential V_i is a site-independent random quantity, with a uniform box disorder distribution, $p(V) = \frac{1}{W} \Theta(\frac{W}{2} - |V|)$.

We focus on the disorder averaged Green function

$$\langle G_k(w) \rangle_{av} = - \frac{\delta}{\delta \eta_{wk}} \langle \ln Z(V_i, \eta_{wk}) \rangle_{av} |_{\eta_{wk}=0}, \quad (2)$$

with $\langle (\dots) \rangle_{av} = \int dV p(V) (\dots)$ standing for the disorder averaging, and η_{wk} is a source field.

In the replica method, one employs the relation $\ln Z = \lim_{m \rightarrow 0} \frac{Z^m - 1}{m}$, with m being the number of replicas. Hence, the above Green function can be written in terms of m powers of Z which is much more tractable than a logarithm. Using Grassmann functional integrals for quantum averaging, and the replica method for disorder averaging, one can rewrite Eq. (2)

as ($\mathcal{D}c \equiv \prod_{wk\alpha} dc_{wk}^\alpha$, α the replica index)

$$\langle G_k(w) \rangle_{av} = - \lim_{m \rightarrow 0} \frac{1}{m} \frac{\delta}{\delta \eta_{wk}} \left\langle \int \mathcal{D}\bar{c} \mathcal{D}c e^{-S[c^\alpha, \bar{c}^\alpha]} \right\rangle_{av} \Big|_{\eta_{wk}=0}, \quad (3)$$

with the lattice action

$$S = \sum_{wk\alpha} \bar{c}_{wk}^\alpha (-i w_n + \varepsilon_k - \mu + \eta_{wk}) c_{wk}^\alpha + \sum_{i\alpha} V_i \int_0^\beta d\tau n_i^\alpha(\tau), \quad (4)$$

where $w_n = (2n+1)\pi T$. Averaging over the distribution $p(V)$ in Eq. (4), we obtain

$$S = \sum_{wk\alpha} \bar{c}_{wk}^\alpha (-i w_n + \varepsilon_k - \mu + \eta_{wk}) c_{wk}^\alpha + \sum_i W(\tilde{n}_i), \quad (5)$$

where $W(\tilde{n}_i)$ is the elastic effective interaction between electrons of different replicas, and may be expressed through cumulants $\langle V^l \rangle_c$ as [4]

$$\begin{aligned} e^{-W(\tilde{n}_i)} &= \int dV_i p(V_i) e^{-V_i \sum_\alpha \int d\tau n_i^\alpha(\tau)} \\ &= e^{-\sum_{l=2}^\infty \frac{1}{l!} \langle V^l \rangle_c (\sum_\alpha \int d\tau n_i^\alpha(\tau))^l}. \end{aligned} \quad (6)$$

Following the DF procedure of [6], we introduce an effective single-site impurity reference problem by rewriting the original action as

$$S = \sum_i S_{imp}[c^\alpha, \bar{c}^\alpha] - \sum_{wk\alpha} \bar{c}_{wk}^\alpha (\Delta_w - \varepsilon_k - \eta_{wk}) c_{wk}^\alpha, \quad (7)$$

with an effective impurity action

$$S_{imp} = \sum_{\alpha w} \bar{c}_{iw}^\alpha (-i w - \mu + \Delta_w) c_{iw}^\alpha + W(\tilde{n}_i), \quad (8)$$

where Δ_w is a local, and yet unknown, hybridization function describing the interaction of the impurity with the effective medium. Our goal is to express the Green function and other properties of the original lattice via the quantities of such impurity problem.

So far we have moved the local part of the lattice action to the effective impurity. One can go further and transfer the non-local part of the action to the auxiliary degrees of freedom, so that the original real fermions carry information about the local part only. In the DF scheme [6] this is done by introducing the auxiliary dual fermions via Gaussian transformation of the non-local part of Eq. (7), i.e.,

$$e^{\bar{c}_{wk}^\alpha A_{wk}^2 c_{wk}^\alpha} = \frac{A_{wk}^2}{\lambda_w^2} \int \mathcal{D}\bar{f} \mathcal{D}f e^{-\lambda_w (\bar{c}_{wk}^\alpha f_{wk}^\alpha + \bar{f}_{wk}^\alpha c_{wk}^\alpha) - \frac{\lambda_w^2}{A_{wk}^2} \bar{f}_{wk}^\alpha f_{wk}^\alpha} \quad (9)$$

with $A_{wk}^2 = (\Delta_w - \varepsilon_k - \eta_{wk})$, and λ_w yet to be specified.

With such a transformation, the lattice Green function of Eq. (3) can be rewritten as

$$\langle G_k(w) \rangle_{av} = - \lim_{m \rightarrow 0} \frac{1}{m} \frac{\delta}{\delta \eta_{wk}} \frac{(\Delta_w - \varepsilon_k - \eta_{wk})}{\lambda_w^2}$$

$$\begin{aligned} &\times \int \mathcal{D}\bar{f} \mathcal{D}f e^{-\sum_{wk\alpha} \lambda_w^2 \bar{f}_{wk}^\alpha (\Delta_w - \varepsilon_k - \eta_{wk})^{-1} f_{wk}^\alpha} \\ &\times \int \mathcal{D}\bar{c} \mathcal{D}c e^{-\sum_i S_{site}^i[\bar{c}_i^\alpha, c_i^\alpha; \bar{f}_i^\alpha, f_i^\alpha]} \Big|_{\eta_{wk}=0}, \end{aligned} \quad (10)$$

in which the replicated site action for site i is of the form

$$S_{site}^i = S_{imp} + \sum_{\alpha w} \lambda_w (\bar{c}_{iw}^\alpha f_{iw}^\alpha + \bar{f}_{iw}^\alpha c_{iw}^\alpha). \quad (11)$$

The inter-site coupling in Eq. (10) has been transferred to a coupling between dual fermions. This allows us to integrate out the real fermion degrees of freedom from the local site action S_{site}^i for each site i separately, i.e.,

$$\begin{aligned} &\int \prod_{\alpha w} d\bar{c}_i^\alpha d c_i^\alpha e^{-S_{site}^i[\bar{c}_i^\alpha, c_i^\alpha; \bar{f}_i^\alpha, f_i^\alpha]} \\ &= Z_{imp} e^{-\sum_{w\alpha} \lambda_w^2 g_{imp}^\alpha(w) \bar{f}_{iw}^\alpha f_{iw}^\alpha - \sum_{\alpha\beta} V_{d,i}^{\alpha,\beta} [\bar{f}_i^\alpha, f_i^\beta]} \end{aligned} \quad (12)$$

in which Z_{imp} is the partition function for the replicated impurity system. As in the clean case [6], formally this can be done up to infinite order, which makes mapping to DF *exact*. Choosing for convenience $\lambda_w = g_{imp}^\alpha(w)^{-1}$, the lowest-order of the replicated non-antisymmetrized DF potential $V_{d,i}^{\alpha,\beta} [\bar{f}_i^\alpha, f_i^\beta]$ reads as

$$V_{d,i}^{\alpha,\beta} [\bar{f}_i^\alpha, f_i^\beta] = \frac{1}{2} \sum_{ww'} \gamma^{\alpha,\beta}(w, w') \bar{f}_{iw}^\alpha \bar{f}_{iw'}^\beta f_{iw'}^\beta f_{iw}^\alpha, \quad (13)$$

where the CPA full vertex

$$\gamma^{\alpha,\beta}(w, w') = \frac{-\chi_{imp}^{\alpha\beta}(w, w') - \chi_{0,imp}^{\alpha\beta}(w, w')}{[g_{imp}^\alpha(w) g_{imp}^\beta(w')]^2}, \quad (14)$$

$$\chi_{0,imp}^{\alpha\beta}(w, w') = -g_{imp}^\alpha(w) g_{imp}^\beta(w'), \quad (15)$$

with $g_{imp}^\alpha(w) = - \int \mathcal{D}\bar{c} \mathcal{D}c e^{-S_{imp}} c_w^\alpha \bar{c}_w^\alpha$ and $\chi_{imp}^{\alpha\beta}(w, w') = \int \mathcal{D}\bar{c} \mathcal{D}c e^{-S_{imp}} c_w^\alpha c_{w'}^\beta \bar{c}_{w'}^\beta \bar{c}_w^\alpha$ being the impurity averaged single- and two-particle Green functions, respectively.

After taking the derivative with respect to the source field η_{wk} , the Green function of Eq. (10) reads as

$$\langle G_k(w) \rangle_{av} = (\Delta_w - \varepsilon_k)^{-1} + \frac{\langle G_{d,k}(w) \rangle_{av}}{[(\Delta_w - \varepsilon_k) g_{imp}^\alpha(w)]^2}, \quad (16)$$

where we define the averaged DF Green function as

$$\begin{aligned} \langle G_{d,k}(w) \rangle_{av} &= - \lim_{m \rightarrow 0} \frac{1}{m} \sum_{\alpha'} \int \mathcal{D}\bar{f} \mathcal{D}f e^{-\sum_{wk\alpha} S_d^0} \\ &\times e^{-\sum_{i\alpha\beta} V_{d,i}^{\alpha,\beta} [\bar{f}_i^\alpha, f_i^\beta]} f_{wk}^{\alpha'} \bar{f}_{wk}^{\alpha'}, \end{aligned} \quad (17)$$

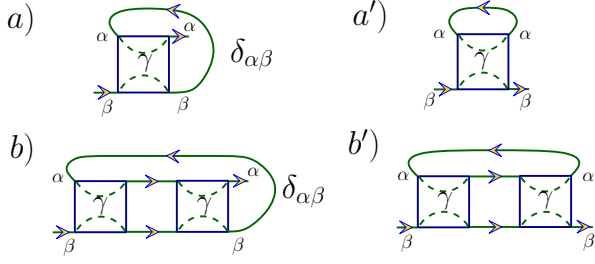


FIG. 1: (color online) First and second order DF self-energy diagrams. All diagrams with scattering of electrons along a closed loop, e.g. a' and b' , vanish in the replica limit. Here, γ is the CPA full vertex, with conserved frequency indicated by dashed lines and α and β the replica.

and $S_d^0 = \bar{f}_{wk}^\alpha \left[\frac{(\Delta_w - \varepsilon_k)^{-1} + g_{imp}^\alpha(w)}{g_{imp}^\alpha(w)^2} \right] f_{wk}^\alpha$ is the non-interacting DF action.

To calculate the DF Green function of Eq. (17), we use diagrammatic perturbation theory. Here the non-trivial and crucial difference between the disordered and clean cases is that the interaction between replicas is off-diagonal, which puts certain constraints on the topology of Green function graphs. In particular, all graphs with closed fermion loops vanish (Fig. 1). This is because each closed fermion loop contains one free replica summation which gives an extra factor of m in Eq. (17), and thus equals to zero when $m \rightarrow 0$ [11].

Single-particle properties.— We first present the single-particle Green function for a one-dimensional lattice. After solving the impurity part, one obtains the averaged impurity Green function $g_{imp}(w) = \int dV p(V) \frac{1}{iw_n + \mu - \Delta(w) - V}$ and corresponding impurity vertex γ . Then, the DF part is solved self-consistently using standard diagrammatic perturbation theory. Next, the real lattice Green function from Eq. (17) is recalculated, and new hybridization function $\Delta(w)$ is constructed to parametrize the impurity problem. This is repeated until self-consistency is reached, namely $\sum_k G_{d,k}(w) = 0$, with all local diagrams (e.g. diagram a in Fig. 1) being zero.

In Fig. 2 we present results for single-particle Green function obtained from a fully self-consistent infinite ladder diagram summation (in both particle-hole (p-h) and particle-particle (p-p) channels) for the DF self-energy. To consider the effect of non-local correlations, we compare our DF results with CPA and DCA results for cluster size $N_c = 20$. The local Matsubara Green function (left panel) shows that inclusion of inter-site correlations leads to corrections to the CPA Green function. Both DF and DCA results show good agreement at small and large disorder strength. The local density of states (DOS) (right panel) also displays satisfactory agreement between DF and DCA results. Indeed, for weak disorder

($W = 0.25$), the results from CPA, DCA and DF calculations are practically the same. As the disorder strength increases, the non-local corrections become important (with finite momentum dependence of the self-energy) and the differences between the CPA and DF DOS are more pronounced. The DF successfully captures such correlations by producing additional features [5] which are also in good agreement with the fully converged DCA result, especially for large disorder strength ($W = 2.0$).

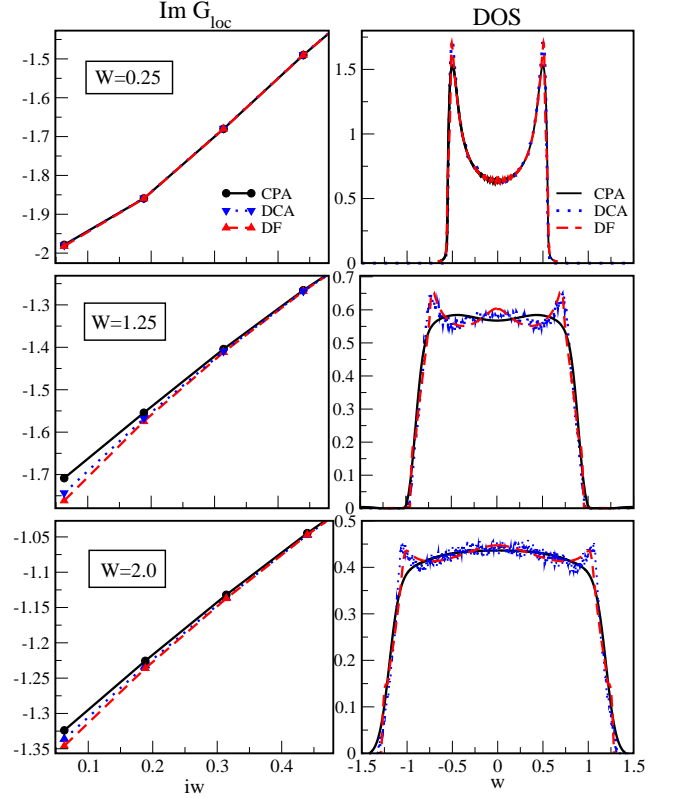


FIG. 2: (color online) The imaginary part of the local Matsubara Green function at $T = 0.02$ (left) and the total density of states (right) for different disorder strengths: $W = 0.25, 1.25, 2.0$ ($4t = 1$). For comparison, we present data obtained within CPA, a finite cluster DCA ($N_c = 20$) and DF methods. Inclusion of inter-site correlations leads to corrections to the CPA Green function (left panel) and appearance of additional structures at larger disorder in the total density of states (right panel). In each case, the DF captures the features of the DCA density of states and is in nearly exact agreement for the Green function.

Two-particle properties.— Although the CPA provides a good qualitative description of single-particle quantities, it fails to capture Anderson localization because the two-particle vertex does not depend on the transfer momentum between incoming and outgoing particles. Thus, the conductivity reduces to the bare p-h bubble so that vertex corrections are ignored [12, 13].

In our scheme, the full vertex is non-local, so we expect

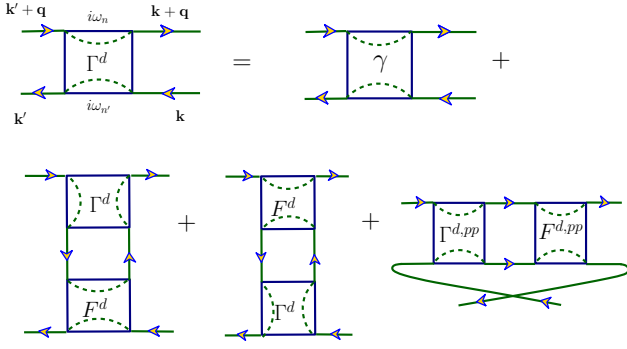


FIG. 3: (color online) Irreducible DF p-h horizontal vertex Γ^d is calculated using parquet equation with crossing contributions from p-h “vertical” and p-p channels. The fully irreducible vertex is approximated by γ . $\Gamma^{d,pp}$ and $F^{d,pp}$ are the irreducible and full p-p vertices, respectively.

to obtain finite vertex corrections describing “weak” localization effects [14]. As our formalism is best converged on Matsubara frequency, we calculate the low temperature dc conductivity following [15] as

$$\sigma_{dc} = \frac{\beta^2}{\pi} \Lambda_{xx} \left(\mathbf{q} = 0, \tau = \frac{\beta}{2} \right), \quad (18)$$

$\beta = 1/k_B T$, and current-current correlation function $\Lambda_{xx}(\mathbf{q}, \tau) = \langle j_x(\mathbf{q}, \tau) j_x(-\mathbf{q}, 0) \rangle$. To obtain this lattice correlation function, one needs to calculate the DF two-particle Green function $\chi^d = -\chi_0^d - \chi_0^d F^d \chi_0^d$, with $\chi_0^d = G^d G^d$ [6]. For the disordered case, one has to remember that in the DF vertex F^d all diagrams containing closed loops are zero.

As usual, F^d is obtained from the Bethe-Salpeter equation $F^d = \Gamma^d + \Gamma^d \chi_0^d F^d$, where Γ^d is the irreducible DF vertex in the p-h horizontal channel (c.f. Fig. 3). To calculate the last quantity, we use the parquet equations which account for the crossing contributions from the p-p and the “vertical” p-h channels [9]. Here the fully irreducible vertex is approximated by the impurity full vertex γ . This procedure allows us to incorporate the important maximally-crossed diagrams [12]. The conductivity can be decomposed into two parts, $\sigma = \sigma_0 + \Delta\sigma$, where σ_0 is the mean-field Drude conductivity, coming from the bare bubble χ_0 , and the second part $\Delta\sigma$ incorporates the vertex corrections.

Our results for the dc conductivity in dimensions $d = 1$ and $d = 2$ are presented in Fig. 4. The data show that the disorder DF method is able to capture weak localization with vertex corrections (vanishing in CPA) leading to a net decrease of conductivity. In $d = 1$, as the disorder strength increases, the DF vertex corrections are more pronounced, while in $d = 2$ they are much weaker, as expected [14].

Conclusions.— We generalize the DF approach to include disordered non-interacting systems using the

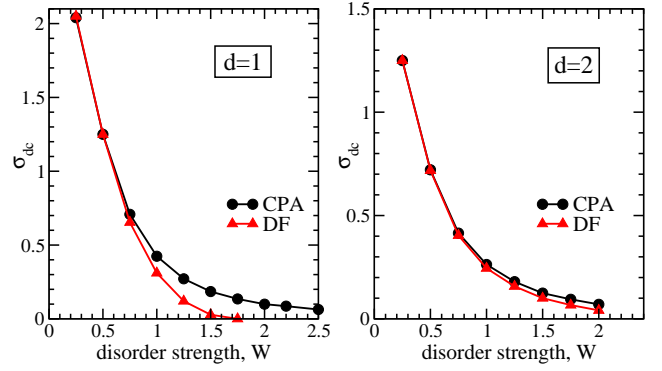


FIG. 4: (color online) Conductivity as function of disorder strength using CPA and DF methods is shown. Data are obtained for $d = 1$ and $d = 2$ at $T = 0.02$. Our results show that vertex corrections incorporated in DF approach allow to capture weak localization leading to the decrease of the net conductivity.

replica method. Our formalism incorporates non-local disorder-induced correlations neglected in the single-site CPA. While in the DCA the multi-scattering effects are limited by the size of the cluster, our method allows us to treat spatial correlations on all length scales. Comparing our results with large-cluster DCA data, we find rather good agreement. This shows that the DF scheme presents a powerful alternative to the existing cluster theories for description of non-local physics in disordered systems. More significantly, our method incorporates finite weak localization corrections to the mean-field conductivity - the precursor effect of Anderson localization. We believe that the DF disorder scheme traces a clear avenue to study a wide variety of physical phenomena, including the interplay of weak localization effects and strong electron interactions, which may be treated on equal footing in our method. Work on this direction and generalization to cluster cases [16] are in progress. As a promising candidate to replace CPA, its application to study non-local effects in electronic structure calculations is also envisioned.

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